Supporting Information

Free H_2 Rotation vs Jahn-Teller Constraints in the Non-Classical Trigonal (TBP)Co-H_2 Complex

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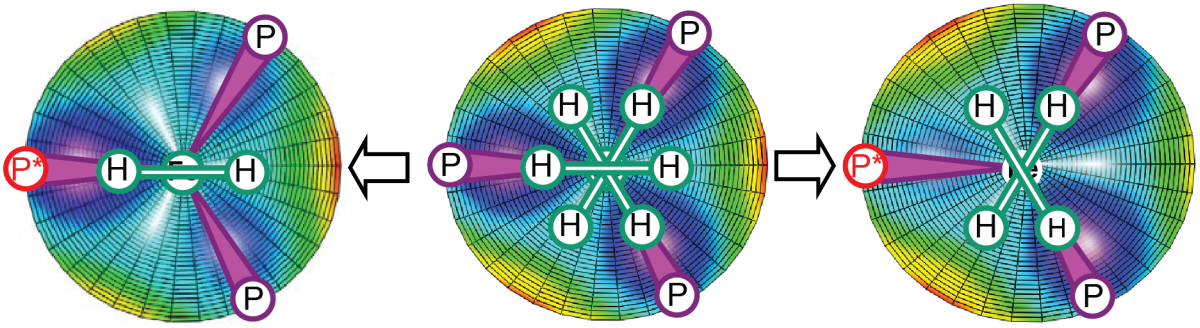

Figure S1: Schematic representation of the C_3 APES for H_2 orientation of a trigonal M-H_2 complex (***center***) and with JT distortion along one M-P bond, which can create a global minimum (***left***) or maximum (***right***) along the bond. The cross product of C_3 with the C_2 symmetry of H_2 π rotation yields the C_6 APES of **Fig 7**.

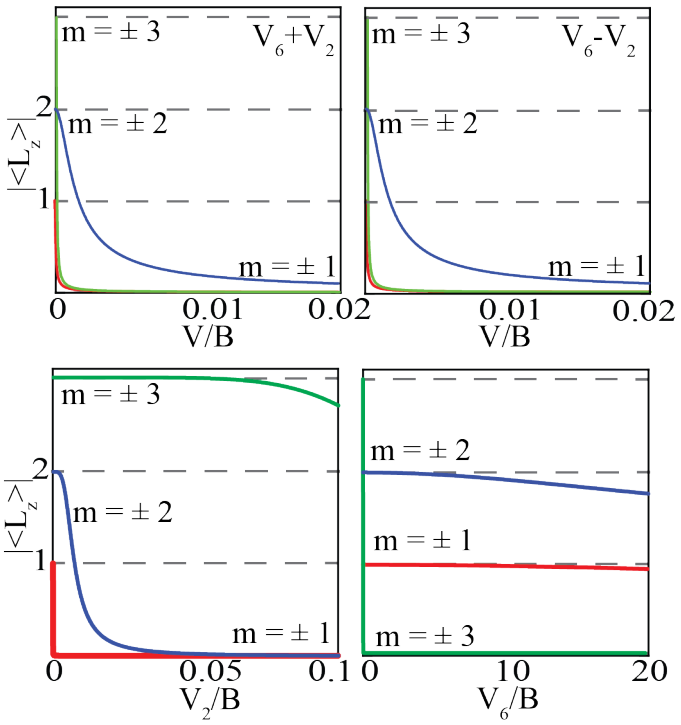

Figure S2: Expectation value of rotational angular momentum $<L_z>$ as a function of V_n/B for two-fold symmetry (n=2) (***left***) and six-fold symmetry (n=6) (***right***)

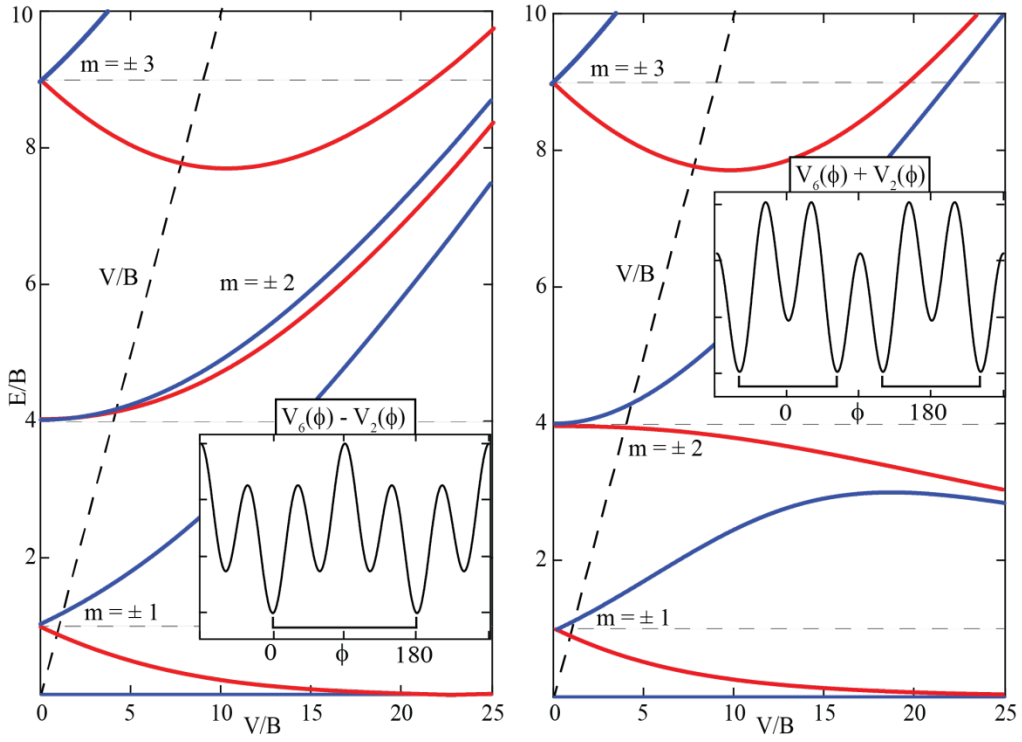

Figure S3: Energy levels for M-H_2 complexes with six-fold symmetric potential, V_6, with additional distortion that introduces a two-fold potential with $V_2 = 0.5\ V_6$, with the subtraction of the two-fold potential (**left**) leaving a pair of minima or addition (**right**) leaving two pairs of minima The resulting potentials are shown as insets. Energies are plotted in units of B. Anti-symmetric states are shown in blue lines and symmetric states are shown in red lines.